A NOTE ON THE OSCILLATING ROTATOR

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ABSTRACT. The problem of the oscillating rotator has been solved from the standpoint of Sonine's polynomials developed by the author recently.

1. The problem was first treated wave-mechanically by Fues (1926) and later by Sommerfeld (1930) considering the rotator oscillating in space and obeying the Kratzer-form of the potential energy. But the problem was hardly solved in its entirety on account of mathematical difficulty in attacking the perturbations involved in calculating the eigenvalue. Chakravarti (1938), handled the problem from the standpoint of perturbation calculations and expanded the eigenfunctions in terms of the Hermitean polynomials and calculated the dissociation energy for the diatomic molecules BeH, CdH, C_2 and N_2. In the next section I shall point out his method of approach to the problem. But in the present paper I am going to deal with it from the standpoint of Sonine's polynomials developed by me recently (Basu, 1943).

2. The wave equation we have to tackle is the following (*vide* Sommerfeld, *l.c.*, p. 28.):

$$\frac{d^2F}{d\rho^2}-\frac{m(m+1)}{\rho^2}F+\frac{8\pi^2 I}{h^2}(E-U)F=0 \qquad \dots \quad (1)$$

where $J=\mu r_e^2$ ($\mu=$ reduced mass of the diatomic molecule, $r=$ the mean distance between the two nuclei), $\rho=r/r_e$, and Kratzer gives

$$U(\rho)=A-J\omega_0^2\left\{\frac{1}{\rho}-\frac{1}{2\rho^2}+b(\rho-1)^3+c(\rho-1)^4+\dots\right\} \qquad (2)$$

wherein $\omega_0=$ frequency of small vibration of the oscillator if the small terms b, c,... were absent.

Chakravarti and Fues made a transformation by putting $\zeta=\rho-1$, and in the resulting equation expanded $m(m+1)/(1+\zeta)^2$ in ascending powers of ζ ($<<1$), in order to avoid a three-term sequence relation amongst the successive coefficients of the polynomial form of the eigenfunction (Sommerfeld, *l.c.*, p. 27), but we can tackle the problem as it stands without any such transformation and expansion.

For the zero-order approximation neglect b, c,... and get

$$\frac{d^2f}{d\rho^2}+\left\{-\beta_0^2+\alpha^2\left(\frac{2}{\rho}-\frac{1}{\rho^2}\right)-\frac{m(m+1)}{\rho^2}\right\}f=0 \qquad \dots \quad (3)$$

where $\beta^2=\dfrac{8\pi^2 J}{h^2}(A-E)$, $\alpha=2\pi J\omega_0/h(>>1)$, $\beta=\beta_0(b,\ c,\dots=0)$, $F=f$.

Considering the asymptotic behaviour of f, *viz.*, $f \sim e^{\pm\beta_0\rho}$ and rejecting *plus* sign, we see $f = e^{-\beta_0\rho}v(\rho)$ where

$$v'' - 2\beta_0 v' + \left[\alpha^2\left(\frac{2}{\rho} - \frac{1}{\rho^2}\right) - \frac{m(m+1)}{\rho^2}\right]v = 0. \quad \ldots \quad (4)$$

For the polynomial type of solution of $v(\rho)$, the index γ is given by

$$\gamma(\gamma-1) = m(m+1) + \alpha^2, \text{ or } \gamma = \tfrac{1}{2} \pm \sqrt{(m+1/2)^2 + \alpha^2}.$$

We should take *plus* sign before the radical in order that γ may be positive and finite for $\rho = 0$.

Next put $v(\rho) = \rho^\gamma u$ and obtain the $u(\rho)$ equation as

$$\rho u'' + (2\gamma - 2\beta_0\rho)u' + 2(\alpha^2 - \beta_0\gamma)u = 0, \quad \ldots \quad (5)$$

which, when transformed by $z = 2\beta_0\rho$, stands thus

$$z\frac{d^2u}{dz^2} + (2\gamma - z)\frac{du}{dz} + nu = 0, \quad \ldots \quad (6)$$

where n (an integer) $= (\alpha^2 - \beta_0\gamma)/\beta_0$ and $u = S^n_{2\gamma}(z)$, a Sonine's polynomial. Hence

$$f \sim e^{-\beta_0\rho}\rho^\gamma S^n_{2\gamma}(z) \sim e^{-\frac{1}{2}z} z^\gamma S^n_{2\gamma}(z). \quad \ldots \quad (7)$$

If N_r be the normalisation factor, the requirement for normalisation is

$N_r^2 \int_0^\infty r^2 f^2 dr = 1$, and remembering $r = \frac{r_e}{2\beta_0} z$, this means

$$N_r^2 \left(\frac{r_e}{2\beta_0}\right)^3 \int_0^\infty e^{-z} z^{2\gamma} S^n_{2\gamma}(z) S^n_{2\gamma}(z) dz = 1. \quad \ldots \quad (8)$$

Now the value of the integral (Basu, *l.c.*)

$$= 2(n+\gamma).n![\Gamma(2\gamma)]^2/\Gamma(n+2\gamma).$$

Hence

$$N_r = 2\left(\frac{\beta_0}{r_e}\right)^{\frac{3}{2}} \left\{\frac{\Gamma(n+2\gamma)}{(n+\gamma).n!}\right\}^{\frac{1}{2}} \Big/ \Gamma(2\gamma). \quad \ldots \quad (9)$$

From (6), $\beta_0 = \alpha^2/(n+\gamma)$,

$$\therefore \quad N_r = \frac{2\alpha^3}{r_e^{\frac{3}{2}}} \frac{1}{(n+\gamma)^2\Gamma(2\gamma)} \sqrt{\frac{\Gamma(2\gamma+n)}{n!}}, \quad \ldots \quad (10)$$

From this value of β_0, the energy-value $E = E_0$ was calculated by Sommerfeld and Fues by the usual polynomial method.

3. Retaining $b, c, \ldots$ terms in Eq. 1, analogous procedure gives

$$\frac{d^2F}{d\rho^2} + \left\{-\beta^2 + \alpha^2\left(\frac{2}{\rho} - \frac{1}{\rho^2}\right) - \frac{m(m+1)}{\rho^2}\right\}F = -2\alpha^2[b(\rho-1)^3 + c(\rho-1)^4]F\ldots \quad (11)$$

wherein, we have ignored $(\rho-1)^5$ and other higher order terms.

Suppose $F = e^{-\beta\rho}v(\rho) = e^{-\beta\rho}\rho^\gamma U(\rho)$, where γ will have the same value as before. The $U(\rho)$-equation becomes (by putting $z = 2\beta\rho$)

$$z\frac{d^2U}{dz^2} + (2\gamma - z)\frac{dU}{dz} + NU = (f_1 z + f_2 z^2 + \ldots + f_5 z^5)U \quad \ldots \quad (12)$$

where $f_1 = \alpha^2(b-c)/2\beta_0^2$, $f_2 = -\alpha^2(3b-4c)/4\beta_0^3$, $f_3 = 3\alpha^2(b-2c)/8\beta_0^4$,

$f_4 = -\alpha^2(b-4c)/16\beta_0^5$, $f_5 = -\alpha^2 c/32\beta_0^6$; $N = (\alpha^2 - \beta\gamma)/\beta$.

Put $U = u + \eta$. $N = n + \epsilon$ and obtain by substitution in (12) the following perturbed equation (rejecting small quantities $f_1\eta$, etc. and $\epsilon\eta$) :

$$z\frac{d^2\eta}{dZ^2} + (2\gamma - z)\frac{d\eta}{dz} + n\eta = [-\epsilon + (f_1 z + \ \dots \ + f_5 z^5)]u. \qquad \dots \quad (13)$$

It is to be noted that

$$\beta = \frac{\alpha^2}{n+\gamma+\epsilon} = \frac{\alpha^2}{n+\gamma}\left(1 - \frac{\epsilon}{n+\gamma}\right) = \beta_0\left(1 - \frac{\epsilon}{n+\gamma}\right). \qquad \dots \quad (14)$$

Suppose $$\eta = \sum_l C_l S^l_{2\gamma}(z). \qquad \dots \quad (15)$$

Substitution in (13) gives

$$\sum_l (n-l) C_l S^l_{2\gamma}(z) = -[-\epsilon + (f_1 z + \dots)] S^n_{2\gamma}(z). \qquad \dots \quad (16)$$

Multiply both sides by $e^{-z} z^{2\gamma-1} S^l_{2\gamma}(z)$ and integrate between $z = 0$ to ∞. This gives (*vide* Basu, *l.c.*)

$$C_l \times \frac{n![\Gamma(2\gamma)]^2}{\Gamma(n+2\gamma)} = \frac{1}{n-l}\int_0^\infty [\epsilon - (f_1 z + \dots)] S^n_{2\gamma}(z) S^l_{2\gamma}(z) e^{-z} z^{2\gamma-1} dz,$$

and consequently C_l (coefficients of the perturbed eigenfunction η) can be found out by evaluating the right-hand member, subject to the condition that C_n is to remain finite (notwithstanding $n = l$ makes the denominator $= 0$). This requires

$$\int_0^\infty [\epsilon - (f_1 z + \dots)] e^{-z} z^{2\gamma-1} S^n_{2\gamma}(z) S^n_{2\gamma}(z) dz = 0 \qquad \dots \quad (17)$$

or $$\epsilon . \frac{n![\Gamma(2\gamma)]^2}{\Gamma(2\gamma+n)} = f_1\{A\} + f_2\{B\} + f_3\{C\} + f_4\{D\} + f_5\{E\} \qquad \dots \quad (18)$$

where $$\{A\} = \int_0^\infty e^{-z} z^{2\gamma} S^n_{2\gamma}(z) S^n_{2\gamma}(z) dz = \frac{n![\Gamma(2\gamma)]^2}{\Gamma(n+2\gamma)} g_1(n, \gamma);$$

$$\{B\} = \int_0^\infty e^{-z} z^{2\gamma+1} S^n_{2\gamma}(z) S^n_{2\gamma}(z) dz = \frac{n![\Gamma(2\gamma)]^2}{\Gamma(n+2\gamma)} g_2(n, \gamma);$$

$$\{C\} = \int_0^\infty e^{-z} z^{2\gamma+2} S^n_{2\gamma}(z) S^n_{2\gamma}(z) dz = \frac{n![\Gamma(2\gamma)]^2}{\Gamma(n+2\gamma)} g_3(n, \gamma);$$

$$\{D\} = \int_0^\infty e^{-z} z^{2\gamma+3} S^n_{2\gamma}(z) S^n_{2\gamma}(z) dz = \frac{n![\Gamma(2\gamma)]^2}{\Gamma(n+2\gamma)} g_4(n, \gamma);$$

$$\{E\} = \int_0^\infty e^{-z} z^{2\gamma+4} S^n_{2\gamma}(z) S^n_{2\gamma}(z) dz = \frac{n![\Gamma(2\gamma)]^2}{\Gamma(n+2\gamma)} g_5(n, \gamma);$$

wherein, for brevity, we have written the g's for the following :—

$$
\begin{aligned}
g_1 &= 2(n+\gamma)\,; \\
g_2 &= (n+2\gamma+1)(n+2\gamma)+4n(n+2\gamma)+n(n-1)\,; \\
g_3 &= (n+2\gamma+2)(n+2\gamma+1)(n+2\gamma)+9n(n+2\gamma+1)(n+2\gamma)+9n(n-1)(n+2\gamma) \\
&\quad + n(n-1)(n-2)\,; \\
g_4 &= (n+2\gamma+3)(n+2\gamma+2)(n+2\gamma+1)(n+2\gamma)+16n(n+2\gamma+2)(n+2\gamma+1)(n+2\gamma) \\
&\quad + 36n(n-1)(n+2\gamma+1)(n+2\gamma)+16n(n-1)(n-2)(n+2\gamma) \\
&\quad + n(n-1)(n-2)(n-3)\,; \\
g_5 &= (n+2\gamma+4)(n+2\gamma+3)(n+2\gamma+2)(n+2\gamma+1)(n+2\gamma)+25n(n+2\gamma+3) \\
&\quad (n+2\gamma+2)(n+2\gamma+1)(n+2\gamma)+100n(n-1)(n+2\gamma+2)(n+2\gamma+1)(n+2\gamma) \\
&\quad + 100n(n-1)(n-2)(n+2\gamma+1)(n+2\gamma) + 25n(n-1)(n-2)(n-3)(n+2\gamma) \\
&\quad + n(n-1)(n-2)(n-3)(n-4). \qquad \dots \quad (19)
\end{aligned}
$$

Since $\Lambda - \mathrm{E} = \dfrac{h^2}{8\pi^2 \mathrm{J}}\left(\beta_0^2 - \dfrac{2\beta_0^3}{a^2}\epsilon\right)$ [from (3) and (4)], and

$$\epsilon = f_1 g_1 + f_2 g_2 + \dots + f_5 g_5 \quad \text{[from (18)]}$$

we get $\mathrm{E} = \mathrm{E}_0 + \dfrac{h^2}{4\pi^2 \mathrm{J}}\dfrac{\beta_0^3}{a^2}\epsilon = \mathrm{E}_0 + \mathrm{E}_1$, say,

where E_0 (for the unperturbed state $b = c = .. 0$) was obtained by Fues and Sommerfeld, and the additional energy-value ($b \neq 0$, $c \neq 0$) is given by

$$
\begin{aligned}
\mathrm{E}_1 = \frac{h^2}{4\pi^2 \mathrm{J}}\Big\{ & \beta_0(b-c)(n+\gamma) - \tfrac{1}{4}(3b-4c)g_2(n,\gamma) + \frac{3}{8\beta_0}(b-2c)g_3(n,\gamma) \\
& - \frac{1}{16\beta_0^2}(b-4c)g_4(n,\gamma) - \frac{c}{32\beta_0^3}g_5(n,\gamma)\Big\}, \qquad \dots \quad (20)
\end{aligned}
$$

where $\beta_0 = \dfrac{2\pi \mathrm{J}\omega_0}{h}\left\{1 - \tfrac{1}{2}\left(\dfrac{m+\frac{1}{2}}{a}\right)^2 - \dfrac{n+\frac{1}{2}}{a} + \dots\right\}$, $a = 2\pi \mathrm{J}\omega_0/h$.

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